

APR 19 1965

Crops Division
Fort Detrick
Frederick, Md. 21701
'65 April 15

Dear Al (and other notationers):

By this time I hope you have had a chance to relax and exchange some topological gems with Dr. Lederberg.

You may recognize one of the enclosed sheets as a direct copy of a tantalizing "chemicotopological hiatus" (a vacancy in our old analyses) that you posed in 1963. I hope you will give my enclosed tabulation the same bit of attention that we gave your ideas then; in the listed "parenthetical" notations, your added specifications are separated from the old ring marks by the slash, for this pedagogical point: which instructions are easiest?

Howard Bonnett's concern also is my apprehension: we are not topological diagnosticians, and if we cannot deduce correct ring loops from a diagram that reveals all symmetry relations, we are not going to do one bit better by redrawing different kinds of diagrams.

The lookup table (my answer to this hiatus) is well along the way. Just a few hours after I had free time with the BioMath machines, I had an arithmetically closed deck of the first 1330 tricyclic combinations, and by fast sorting had excluded invalid (polynuclear, etc.) combinations.

I really was disturbed by the failure of any of you to see these absolutely infallible simple circuit definitions as I always have seen them. The nonconsecutive line segments are a sharply defined set that begins thus:

AC, AD BD, AE BE CE, AF BF CF DF, AG BG CG DG EG, AH BH CH DH EH FH, etc. ...
1, 2 3, 4 5 6, 7 8 9 10, 11 12 13 14 15, 16 17 18 19 20 21, etc. ...

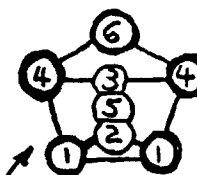
so it is child's play to make checklists from these letter pairs alone.

When you complain that the "locant links" do not show ring sizes, please remind yourselves that these "smallest sets of smallest rings" are pure figments of chemist's minds-- hence trouble. And if we decide first on smallest sums of ring numerals, then on smallest other things, where is there any contradiction such as you implied in your note of August 22, 1963: "The SMALLEST AND FEWEST rings turns out to be impossible-- sometimes you can't have BOTH!" My path-tracers give ALL possible alternatives of longest chains, and alternatives are eliminated by specified minimum measures, no? The only "arbitrary assertions" are these chemically traditional choices, ~~with~~ topological exactness: smallest number of rings, smallest R.N. sum.

If you study the enclosed '65Apr15 tabulation carefully, you will see absolute relations, such as this: Your "enclosed" (underlined) locants are (1) not in the linking recitation if they are intermediate-chain points, or (2) recited only once if they are chain terminals (a or k in this example). Spiro/quadrivalent points also are revealed directly in these recitations. Am I getting through to anyone?

Sincerely yours, Bill

SAMPLE TOPOLOGICAL ANALYSIS OF 8-POINTED HEXABRANCHED PENTAGON:
(Pictured as "8-POINTED TRIANGULAR PRISM" on drawing sheet)
(Forms trigonal prism when bivalent points are removed)



	NONCONSECUTIVE LOCANT LINKS	CORRESPONDING LINE- FORMULA NOTATION	SUM OF FUS.L.	SUM OF RING #	SUMMARY OF RING CIRCUIT-CHECK	PATH IDENTITY BY POINT-TYPES & NO.	DRG #	FINAL RANK
1	AC AF BH EH	(355 B4/G2AF H)	a382	17 =	a3b2c2de2f3g2h2	11253464' = 1	17	17
2	AC AF DG BH	(35 D45/E2AF H)	7	17	a3b2c2d2e2f3g2h	12146435 4	10	11
3	AC BF AH EH	(3 B55 E4/G2BF H)	9	17	a2b3c2de2f3g2h2	11253464" 2	22	24
4	AC DG BF AH	(3 D4 B55/E2BF H)	8	17	a2b3c2d2e2f3g2h	21146435 8	18	20
5	AD AG CH FH	(455 F3/B2AG H)	9	17	a3b2c2d2ef2g3h2	46435211' - 1	25	22
6	AD BF EG AH	(45 E35/H2AG H)	8	17	a3b2cd2e2f2g3h2	34641125 10	19	18
7	AD BF EG CH	(45 E3 B5/A2BF H)	9	17	a2b3c2d2e2f3g2h	64341125 -14	23	23
8	AD CG AH FH	(4 C55 F3/B2CG H)	11	17	a2b2c3d2ef2g3h2	46435211" - 2	28	28
9	AE AF BH DH	(535 B4/C2AB H)	5 *	17	a3b3c2d2e2f2gh2	14641253 7	2	2
10	AE AF CG BH	(535 B4/3ABC H)	5 *	17	a3b3c3de2f2g2h	14352146 6	1	1
11	AE AF CG DH	(535 C4/B2AC H)	6	17	a3b2c3d2e2f2g2h	25341146 9	5	5
12	AE AG CH DH	(545 C3/B2AC H)	6	17	a3b2c3d2e2fg2h2	35214641 - 7	6	6
13	AE BF CH DH	(54 B5 C3/A2BC H)	7	17	a2b3c3d2e2f2gh2	64114352 - 9	13	10
14	AE CF AH BH	(5 C453/D2AE H)	6	17	a3b2c2d2e3f2gh2	11464352 3	7	7
15	AE DF AH CH	(5 D354/B2AE H)	7	17	a3b2c2d2e3f2gh2	46411253 -11	11	12
	(etc., to 30)							

All possible notations are ranked by: (1) ring sum, (2) locant sum, and (3) locant-citing order. '65Mar30/WJW
The cited ring & locant is the SMALLEST & LOWEST going through each newly formed link.
Note that the "point-type" paths occasionally are ambiguous, unlike the "Locant links" and generated notations.

63-8

-2-

- 5) I hope this new analysis may help convince any doubters (hiya, Bill) that my analytic approach to structural formulas via the concept of bridging atoms and multicyclic points is a sound one, for purposes of this notation.
- 6) I believe this analytic approach could be applied to other codes or notations since it is really independent of the particular notation we're using in most ways. Does anybody know how Dyson (oops, I mean the IUPAC notation) handles this problem of WHICH structural formula to encode in compounds like these?

I hope you'll all take the time and trouble to plow through this material. I'm sure there are still loose ends, so please let me know what further difficulties you turn up.

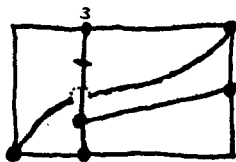
I'll be in Columbus, Ohio from Sunday Aug. 25 through Wed. the 28th doing my bit to present the final report of the NRC project to the parent committee. I know I'll see some of you there. Whether or not I get to go on to the Bureau of Standard's (Tauber's) seminar the next week depends on whether or not Mrs. Brownson and Karl Heumann say it's okay for me to go on there from Columbus (at my own expense) and still charge my return trip ticket from Columbus to San Francisco to the NRC project. I just don't know what the regulations are on this sort of thing. If I do get to stay over, could you and I get together, Bill? Over the Labor Day week end, maybe? Or sometime? There seems to be quite a lot we need to talk over in order to get the manual revision going.

Sincerely,

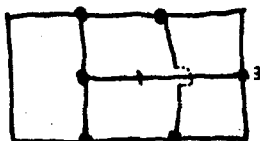
a

Elbert G. Smith

1) JACS 82 5558 (1960)



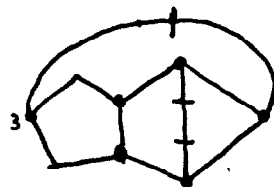
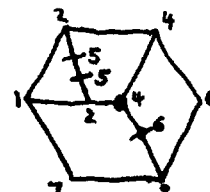
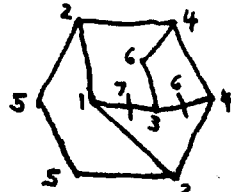
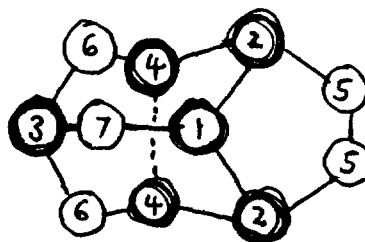
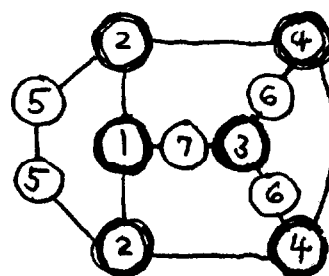
2)



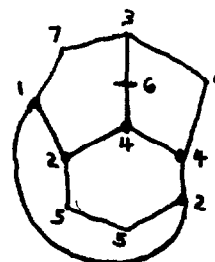
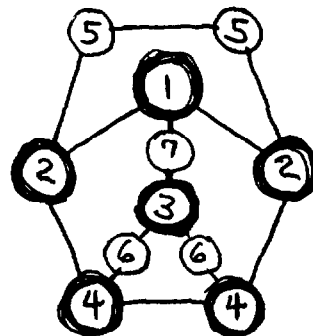
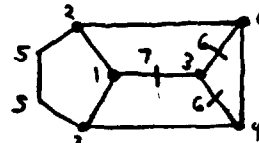
3) Ring Index 4071



4)

WJW: FIRST IDENTIFY KINDS OF POINT-CONNECTIONS:
Apr. 14, 1965

SUGGESTED "ANALYTICAL APPROACH"



just "what the eye can see."

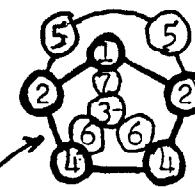
FROM PAGE 1

Aug. 22, 1963

EGS To: any who feel they can successfully encode

(DIFFERENT)

SAMPLE TOPOLOGICAL ANALYSIS OF CONNECTIVITY TABLES FOR A HEXABRANCHED PENTAGON:



	NONCONSECUTIVE LOCANT LINKS	CORRESPONDING LINE- FORMULA NOTATION	SUM OF FUS.L.	SUM OF RING #	SUMMARY OF RING CIRCUIT-CHECK	PATH IDENTITY BY POINT-TYPES	FINAL RANK
1	AE AI DJ GK	(565 G5/H3AEI K)	12	21	= a ₃ bcd ₂ e ₃ fg ₂ h ₂ i ₃ j ₂ k	25521736446' = 2 or -15	8
2	AE AI FJ CK	(5656/4AEF K)	4	22	= a ₄ b ₂ c ₂ d ₂ e ₃ f ₂ gh ₁ i ₃ j ₂ k	46364255217 = 4 -18	11
3	AE BH CK GK	(56 B6 B5/A4BBCH K)	6	22	= a ₂ b ₄ c ₃ d ₂ e ₂ fg ₂ h ₃ i ₁ j ₂ k	64463712552' = 15 - 2	12
4	AE CH BK GK	(5 C6 B6 B5/D4BCCH K)	8	22	= ab ₃ c ₄ d ₂ e ₂ fg ₂ h ₃ i ₁ j ₂ k	64463712552" = 14 - 3	15
5	AE DI AJ GK	(5 D65 G5/H3DEI K)	13	21	= a ₂ bcd ₃ e ₃ fg ₂ h ₂ i ₃ j ₂ k	25521736446 = 3 -14	10
6	AE DI FJ BK	(5 D6 D56/A4DEEF K)	10	22	= a ₂ b ₂ cd ₃ e ₄ f ₃ gh ₁ i ₂ j ₂ k	63644255217 = 8 -17	18
7	AF AI EJ CK	(655 C5/D3AEF K)	6 *	21	= a ₃ bc ₂ d ₂ e ₃ f ₃ gh ₁ i ₂ j ₂ k	17364255246 = 1 -12	1
8	AF BH DI CK	(65 B5 C5/A3BCD K)	7	21	= a ₂ b ₃ c ₃ d ₃ ef ₂ gh ₂ i ₂ j ₂ k	64217364255 = 10 - 7	2
9	AF DH BI CK	(6 D5 B5 B5/E3BCD K)	9	21	= ab ₃ c ₃ d ₃ e ₂ f ₂ gh ₂ i ₂ j ₂ k	71246364255 = 16 - 6	5
10	AF EI AJ CK	(6 E555/B3AEF K)	8	21	= a ₃ b ₂ c ₂ d ₂ e ₃ f ₃ gh ₁ i ₂ j ₂ k	46371255246 = 5 -11	4
11	BF AI CK GK	(B566 B5/A4BBCF K)	6	22	= a ₂ b ₄ c ₃ def ₂ g ₂ h ₁ i ₂ j ₂ k	71255246364 = 18 - 4	13
12	CBF CH AJ GK	(B5 B56 G5/I3BCH K)	12	21	= ab ₃ c ₃ def ₂ g ₂ h ₃ i ₂ j ₂ k	71255244636 = 17 - 8	9
13	BG AI CK FK	(B656 C5/A4BBCG K)	7	22	= a ₂ b ₄ c ₃ def ₂ g ₃ h ₁ i ₂ j ₂ k	64255246371 = 12 - 1	14
14	BG DH AJ CK	(B6 D565/A E F2BG K)	8	22	= a ₂ b ₃ c ₂ d ₂ e ₂ f ₂ g ₃ h ₂ i ₂ j ₂ k	64425521736 = 13 - 9	16
15	CG AI BK FK	(C565 B5/A3BCG K)	7	21	= a ₂ b ₃ c ₃ def ₂ g ₃ h ₁ i ₂ j ₂ k	64255217364 = 11 - 5	3
16	CH AI DJ FK	(665 C5 D5/E3CDH K)	11	21	= abc ₃ d ₃ e ₂ f ₂ gh ₃ i ₂ j ₂ k	55246371246 = 7 -10	7
17	DH AI CJ FK	(D565 C6/A B E2CD K)	9	22	= a ₂ b ₂ c ₃ d ₃ e ₂ f ₂ gh ₂ i ₂ j ₂ k	55246364217 = 6 -16	17
18	DH AI EJ BK	(D56 D55/A3DHI K)	10	21	= a ₂ b ₂ cd ₃ e ₂ fgh ₃ i ₃ j ₂ k	63712552446 = 9 -13	6

All possible notations are ranked by: (1) ring sum, (2) locant sum, and (3) locant-citing order.

'65Ap.15/WJW